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Mapping Long-Range 3D Lithium Diffusion in Solid Electrolytes Using Pulsed-Field Gradient NMR and MD Simulations

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Solid-state lithium-based electrolytes improve safety by replacing flammable liquid solvents with stable, non-volatile solids and by physically suppressing dendrite growth, leading to significantly longer battery life. These properties make them particularly well-suited for long-duration energy storage and other demanding applications.

Lithium-ion transport in solid electrolytes is governed by the topology and dimensionality of diffusion pathways. We combined 7Li pulsed-field gradient NMR (PGSE NMR), molecular dynamics (MD) simulations, and X-ray diffraction with Rietveld refinement to investigate long-range 3D lithium diffusion in the high-temperature hexagonal phase of $LiBH_4$, $LiBH_4$–LiBr composites, and lithium-ion-conducting glass–ceramics (LIGPs).

For $LiBH_4$, XRD–Rietveld analysis confirmed the hexagonal $P6_3mc$ symmetry above the phase transition, providing the structural basis for MD simulations that revealed intertwined lithium diffusion channels along [001] with zig–zag jumps across (001) planes. PGSE NMR quantified anisotropic diffusion with DII> DI. By modeling the powder-averaged diffusion tensor, we developed a 3D diffusion model and analytical expressions linking the principal tensor components to experimentally observed spin–echo attenuation. This integrated approach links crystallographic features to macroscopic transport, providing guidelines for tailoring anisotropy and enhancing Li-ion mobility in advanced solid electrolytes.

Kosma Szutkowski obtained his PhD in Physics in 2006 at Adam Mickiewicz University in Poznan, Poland. Subsequently, he was awarded a postdoctoral fellowship at KTH Royal Institute of Technology in Sweden (2006–2008) working with Peter Stilbs and Istvan Furo. He earned his habilitation in Physics in 2019, and since that time, his research has centered on the applications of pulsed-field gradient NMR (PGSE NMR) for studying molecular and ionic diffusion in a broad range of systems, including surfactant assemblies, proteins, porous materials, and polymers. Recently, his research focus has shifted to solid-state electrolytes, combining PGSE NMR with molecular dynamics simulations and complementary structural methods such as X-ray diffraction and Rietveld refinement.